Theory of InGaBiAs dilute bismide alloys for highly efficient InP-based mid-infrared semiconductor lasers

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***Abstract*—We present a theoretical analysis of the properties and performance of mid-infrared dilute bismide quantum well (QW) lasers grown on InP substrates. We analyse the band structure of strained InGaBiAs alloys and quantify their potential for the development of mid-infrared semiconductor lasers. In addition to identifying the permissible growth combinations for this class of laser structures, we perform a comprehensive analysis of the performance of a series of ideal laser structures. We investigate the variation of key material and device parameters on the alloy composition, QW thickness and epitaxial strain, and on this basis identify optimised laser structures for emission across the 3 – 5 μm wavelength range. Our theoretical analysis suggests that InP-based dilute bismide alloys are an extremely promising candidate material system for the development of highly efficient and temperature stable laser diodes operating in the mid-infrared, and also that this class of laser structures is highly compatible with existing InP-based device architectures.**

I. Introduction

The steadily growing research interest in dilute bismide alloys – III-V alloys containing small fractions of substitutional bismuth (Bi) atoms – has focused primarily on materials grown on GaAs substrates. There has also been some effort aimed at developing dilute bismide alloys on InP substrates, interest in which developed intially due to the potential of Bi incorporation to enhance thermoelectric performance [1]. Recent analysis of the band structure of InGaBiAs alloys has suggested that this material system should have significant potential for the development of mid-infrared light-emitting devices on InP substrates [2]. This is particularly appealing from a technological perspective, given the need for robust and efficient mid-infrared light sources for deployment in a range of sensing applications.

Initial analyses of InGaBiAs alloys have confirmed that Bi incorporation brings about a strong reduction in the band gap (E_g) and increase in the spin-orbit-splitting energy (Δ_{SO}), which makes it possible to access a wide range of mid-infrared wavelengths at modest Bi compositions. Theoretical calculations suggest that a band structure having $\Delta_{\text{SO}} > E_g$ can be obtained in InGaBiAs alloys at Bi compositions $x \lesssim 4\%$ [3], and growth of alloys satisfying this band structure has recently been achieved [4]. This suggests that the non-radiative (Auger) recombination and inter-valence band absorption (IVBA) mechanisms involving the spin-split-off band can be suppressed at significantly lower Bi compositions than on GaAs substrates [2], [3].

We present a theoretical analysis of mid-infrared InGaBiAs QW lasers grown on InP substrates. By analysing the InGaBiAs alloy band structure we identify (i) the ranges of strain and wavelength accessible using this novel class of InP-based heterostructures, and (ii) permissible growth combinations for targeting specific emission wavelengths in the 3 – 5 μm range. This high level overview is accompanied by a systematic theoretical analysis of candidate laser structures. Through this analysis we (i) quantify the flexibility of these heterostructures for band structure engineering, (ii) identify laser structures optimised for performance across a range of wavelengths, and (iii) identify and quantify key trends in the expected device performance as functions of key parameters such as QW thickness, epitaxial strain and wavelength.

Our analysis demonstrates that (i) InGaBiAs is a strong candidate material system for achieving lasing at wavelengths > 3 μm on an InP substrate, (ii) Bi incorporation offers significant potential for band structure engineering leading to high-performance devices, and (iii) InGaBiAs alloys offer several intrinsic benefits compared to competing material and device concepts (e.g., many current technologies in this wavelength range are based on the relatively, compared to InP, expensive and technologically immature GaSb platform). Meanwhile, existing InP-based devices have demonstrated lasing only at wavelengths $\lesssim 3$ μm, and to reach these wavelengths has required the use of non-ideal metamorphic or type-II heterostructures. The reduced Bi compositions required to bring about suppression of the dominant Auger and IVBA loss mechanisms on InP should additionally serve as proof of principle for the development of GaAs-based dilute bismide alloys for highly efficient 1.55 μm semiconductor lasers [5].

II. Theoretical model

Our theoretical model of the InGaBiAs band structure is based on an extended basis set 12-band $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian which directly incorporates Bi composition dependent interactions between the extended valence band edge states of the InGaAs host matrix, and localised Bi-related impurity states which are resonant with the InGaAs valence band. We have previously derived and parametrised this model for GaAs-based Bi-containing alloys, and have subsequently extended this approach by using atomistic supercell calculations to take account of incorporation of Bi into an InGaAs host matrix, including parametrisation of the effects on the alloy band structure of (i) co-alloying of In and Bi, and (ii) growth on, and strain with respect to, InP substrates [3]. Beginning from this detailed model of the band structure, our calculations of the electronic and optical properties of QW laser structures follow the computational approach we have previously applied to the study of GaAs-based dilute bismide QW lasers [5], which directly includes Bi-related band structure effects in the calculation of the optical properties and has been demonstrated to be in excellent, quantitative agreement with experiment [6].

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III. Results

Firstly, we have used our theoretical model to analyse the band structure of strained InGaBiAs alloys grown on InP. The results of this analysis are summarised in Fig. 1, where the dashed black, solid blue and solid red lines denote, respectively, alloy compositions for which the in-plane strain, band gap, and difference between the band gap and spin-orbit-splitting energy are constant. Alloys lying above the $E_g = \Delta_{\text{SO}}$ contour have $\Delta_{\text{SO}} > E_g$, so that the dominant Auger and IVBA loss mechanisms are suppressed [2]. Our calculations indicate that emission at wavelengths > 3 μm can be achieved for modest Bi compositions ($x \lesssim 5\%$) and compressive strains ($\epsilon_{xx} \lesssim 1.5\%$). Our calculations also predict that such alloys have $\Delta_{\text{SO}} > E_g$ and large type-I band offsets with respect to unstrained InGaAs. InGaBiAs QWs should therefore mitigate carrier leakage in addition to enabling suppression of the dominant Auger recombination and IVBA mechanisms, and hence provide efficient, temperature stable laser operation without the need to resort to complicated cascade or metamorphic structures, or type-II or Sb-containing QWs, to facilitate the growth on InP of QWs emitting at wavelengths > 3 μm.

Secondly, we have performed a systematic analysis of QW laser structures designed to emit at 3 – 5 μm. The available parameter space for the design of such structures is extremely large, encompassing wide ranges of alloy compositions, QW thicknesses and epitaxial strains. As such, in order to facilitate the identification of trends in the device performance we have restricted our attention at each wavelength to two sets of laser structures, having: (i) fixed QW thickness and variable strain, and (ii) variable QW thickness and fixed strain. In this manner we are able to directly identify key material trends and their contribution to the overall device performance, and also to quantify the potential to use alloy, heterostructure and strain engineering to optimise the laser performance at a given wavelength. In particular, we focus on the gain characteristics in order to optimise the carrier density and differential gain at threshold – which we seek to minimise and maximise, respectively – and on this basis identify laser structures that should deliver high-speed performance at low injection currents. (See Ref. [7] for details.)

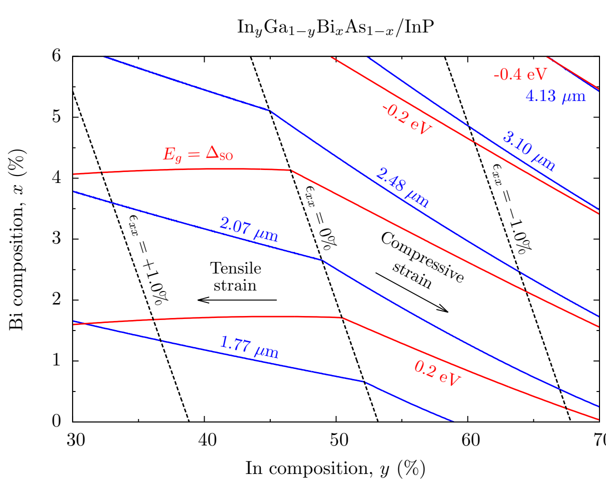

Fig. 1. Composition space map showing the variation of the in-plane strain (ϵ_{xx}, dashed black lines), band gap (E_g, solid blue lines) and difference between the band gap and spin-orbit-splitting energy ($E_g - \Delta_{\text{SO}}$, solid red lines) as a function of Bi and In composition (x and y), for pseudomorphically strained $In_yGa_{1-y}Bi_xAs_{1-x}$ alloys grown on an InP substrate. Incorporation of Bi makes possible the growth of compressively strained type-I QWs having emission wavelengths > 3 μm with $\Delta_{\text{SO}} > E_g$. (See Ref. [7] for details.)

IV. Conclusion

We have developed the theory of the electronic and optical properties of mid-infrared dilute bismide QW lasers grown on InP substrates. Our analysis of the strained InGaBiAs band structure demonstrates that this material system can be used to realise type-I QWs on InP having emission wavelengths > 3 μm, thereby promising to overcome several key limitations associated with current approaches to achieving long-wavelength semiconductor lasers on InP. We further note that > 3 μm emission is achievable in QWs having moderate compressive strains, as well as Bi compositions lying within the range that has already been achieved via epitaxial growth.

Through a systematic analysis of the available design space of InGaBiAs QWs we have quantitatively demonstrated the ability to exploit the impact of Bi on the band structure, in conjunction with heterostructure and strain engineering, to realise optimised laser structures that should deliver highly efficient and temperature stable operation in the 3 – 5 μm wavelength range (via the suppression of the dominant Auger and IVBA loss mechanisms, as well as mitigation of carrier leakage). Overall, our theoretical analysis (i) highlights that dilute bismide alloys offer a promising approach to the development of high-performance InP-based mid-infrared semiconductor lasers, and (ii) explicitly quantifies the potential to develop this novel class of heterostructures in order to deliver enhanced capabilities and performance compared to competing device concepts.

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